

# Umbral Calculus, Difference Equations and the Discrete Schrödinger Equation

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## Abstract

We discuss umbral calculus as a method of systematically discretizing linear differential equations while preserving their point symmetries as well as generalized symmetries. The method is then applied to the Schrödinger equation in order to obtain a realization of nonrelativistic quantum mechanics in discrete space-time. In this approach a quantum system on a lattice has a symmetry algebra isomorphic to that of the continuous case. Moreover, systems that are integrable, superintegrable or exactly solvable preserve these properties in the discrete case.

**Key words:** umbral calculus, difference equations, symmetries, integrability, quantum mechanics, discrete space-time.

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# 1 Introduction

A sizable literature exists on discrete quantum mechanics, that is on quantum mechanics in discrete space–time. We refer to a recent review for motivation and for an extensive list of references [1]. There are many reasons for considering quantum systems in discrete space–time. One is that physical space–time may indeed be discrete, involving an elementary length and some minimal time interval. Then continuous theories would only be approximations to the real world. Another reason is the usual one: on a lattice one can avoid some of the divergence problems occurring in quantum field theories. On the other hand, some properties of quantum systems are lost in any discretization. The aim of this article is to discuss a discretization of space–time in which the Schrödinger equation is replaced by a difference equation. This is done in such a manner that many of the essential properties of the continuous system are preserved. In particular, we preserve the group theoretical and integrability properties of the Schrödinger equation. This is true for the time–dependent, as well as the stationary equation. The free equations, as well as those with potentials, after discretization have symmetry groups, isomorphic to those of the continuous case. Lie point symmetries, after discretization, may however act at several points of the lattice.

Another property that we wish to preserve is that of integrability, and also superintegrability. By integrability, for an  $n$  dimensional quantum system, we mean the existence of  $n$  well defined algebraically independent Hermitian operators  $\{X_1, \dots, X_n\}$  (including the Hamiltonian  $H$ ) commuting pairwise. Superintegrability means that there exist further independent operators,  $\{Y_1, \dots, Y_k\}$ ,  $1 \leq k \leq n - 1$ , commuting with the Hamiltonian  $H$ , but not necessarily with the other operators  $X_i$ , nor  $Y_i$  [2]–[10].

Finally, we wish to preserve exact solvability in the discretization, i.e. the fact that for certain systems (like the harmonic oscillator, or hydrogen atom) it is possible to calculate all energy levels algebraically.

A mathematical tool that we shall use for the study of symmetries and exact solutions of linear equations is the so-called "umbral calculus". This calculus, which originated in 19th century with the work of Sylvester, Cayley and others, was used for a long time as a useful tool to derive combinatorial identities (see, for instance, [11]). Nevertheless, it was only with Rota et al. [12]–[15] that this calculus was put on an axiomatic basis using the language of linear algebra of operators. In Ref. [16], the interested reader can find an up to date survey concerning the origins of umbral calculus

and its many applications in several branches of mathematics, like combinatorics, functional analysis, algebraic topology, theory of special functions and orthogonal polynomials, etc.

Umbral calculus has recently been used explicitly [17], or implicitly [18]–[21], to provide discrete representations of canonical commutation relations, specially in the context of exactly solvable and quasi exactly solvable quantum systems [22]–[24]. Linear differential equations have been discretized in a symmetry preserving manner using commuting difference operators [25]–[27]. An alternative approach [28] to symmetries of linear difference equations makes use of a discretized version of the prolongation theory of evolutionary vector fields. Finally, umbral calculus was used in an implicit manner, to obtain several different symmetry preserving discretizations of the linear heat equation [29].

Symmetries of difference equations, mainly nonlinear ones, have recently received a lot of attention (see e.g. [25]–[39] and references therein). What has emerged for purely difference equations is that in order to capture the essential features and usefulness of symmetries of differential equations it is necessary to make serious adjustments. Either one must go beyond point transformations to generalized ones [32]–[33], or one must use symmetry adapted and transforming lattices (as proposed initially by Dorodnitsyn) [34]–[39].

In this paper we follow the first approach. We consider a fixed lattice and use umbral calculus to obtain symmetries acting simultaneously on more than one point of the lattice. We apply this approach to quantum mechanics.

## 2 Umbral Calculus

To make this article self-contained let us sum up in Section 2.1 some known definitions and also some results proven as theorems by Rota [13], Roman [15] and Dimakis et al. [17].

We shall actually need umbral calculus on spaces of many variables in order to study multidimensional difference equations. However, for simplicity of exposition and notation we shall in this section restrict to the case of one variable  $x$ .

## 2.1 General Theory.

Let  $\mathfrak{F}$  be the algebra of formal power series in a variable  $x$ , and  $\mathcal{P}$  the algebra of polynomials in the same variable. The algebras will be considered over a field  $\mathbb{F}$  of characteristic zero. This field in the subsequent considerations will be identified with  $\mathbb{R}$  or  $\mathbb{C}$ . An element of  $\mathfrak{F}$  is of the form

$$\sum_k a_k x^k \equiv f(x). \quad (2.1)$$

The operations defined in  $\mathfrak{F}$  are the addition of series

$$\sum_{k=0}^{\infty} a_k x^k + \sum_{k=0}^{\infty} b_k x^k = \sum_{k=0}^{\infty} (a_k + b_k) x^k, \quad (2.2)$$

and the multiplication

$$\left( \sum_{k=0}^{\infty} a_k x^k \right) \left( \sum_{l=0}^{\infty} b_l x^l \right) = \sum_{m=0}^{\infty} \left( \sum_{j=0}^m a_j b_{m-j} \right) x^m. \quad (2.3)$$

The algebra  $\mathfrak{F}$  is also called the *umbral algebra* [15].

A polynomial sequence  $p_n(x) \in \mathcal{P}$  is a sequence whose  $n$ -th element is a polynomial of degree  $n$ . We will denote by  $\mathcal{L}$  the algebra of linear operators acting on  $\mathfrak{F}$  or  $\mathcal{P}$ .

**Definition 2.1** A shift operator  $T \in \mathcal{L}$  is a linear operator such that

$$T p(x) = p(x + \sigma), \quad (2.4)$$

where  $p(x)$  is a polynomial and  $\sigma \in \mathbb{F}$ .

**Definition 2.2** An operator  $F \in \mathcal{L}$  is said to be shift-invariant if it commutes with all shift operators (i.e. with  $T$  for all values of  $\sigma$ ).

**Definition 2.3** An operator  $U$  is said to be a delta operator if it is shift-invariant and

$$U x = c \neq 0, \quad (2.5)$$

where  $c \in \mathbb{F}$ .

Using Definition 2.1 and the linearity of shift-invariant operators one can prove the following result. If  $U$  is a delta operator, for every  $c \in \mathbb{F}$  we have

$$U c = 0. \quad (2.6)$$

**Definition 2.4** A polynomial sequence  $p_n(x)$ ,  $n = 0, 1, 2, \dots$ , is called a sequence of basic polynomials for the delta operator  $U$  if

$$p_0(x) = 1, \quad p_n(0) = 0 \quad \forall n > 0, \quad (2.7)$$

and

$$U p_n(x) = n p_{n-1}(x). \quad (2.8)$$

It is easy to show that every delta operator has a unique sequence of basic polynomials. We will denote by  $\mathfrak{I}$  the one-to-one correspondence between basic sequences and delta operators.

Let  $\mathcal{A}$  be the algebra of shift-invariant operators, endowed with the usual operations of sum of two operators, product of a scalar with an operator, and product of two operators. We introduce a multiplication operation  $*$  :  $\mathcal{A} \times \mathcal{L} \rightarrow \mathcal{L}$ , defined by

$$F * O = [F, O] = FO - OF, \quad (2.9)$$

where  $F$  is a shift-invariant operator and  $O \in \mathcal{L}$ . In particular, if  $x$  denotes the multiplication operator  $x : p(x) \rightarrow xp(x)$ , then  $F * x$  corresponds to what in the umbral literature is known as the Pincherle derivative of  $F$ . In this case we will write

$$F' = F * x = [F, x]. \quad (2.10)$$

Using the  $*$  multiplication the Leibnitz rule becomes

$$F * (fg) = (F * f)g + f(F * g) \quad (2.11)$$

and the Jacobi identity is expressed by

$$F * G * H + G * H * F + H * F * G = 0. \quad (2.12)$$

Let us now consider a pair of shift-invariant operators: a *delta* operator  $U \in \mathcal{L}$  and its conjugate operator  $\beta \in \mathcal{L}$ , defined in such a way that the *Heisenberg–Weyl algebra* is satisfied:

$$[U, x\beta] = 1. \quad (2.13)$$

It is possible to prove that, if  $U$  is a delta operator, then the inverse of  $U'$  exists ([13], p. 18). Therefore, the operator  $\beta$  is determined by the relation:

$$\beta = (U')^{-1}. \quad (2.14)$$

To prove this it suffices to notice that

$$1 = [U, x\beta] = [U, x]\beta = U'\beta,$$

where the property  $[U, \beta] = 0$  has been exploited. Eq.(2.14) follows.

Let us present some specific examples of realizations of the conjugate operators  $U$  and  $\beta$  in terms of derivatives and shifts, respectively.

**Example 2.1.** The continuous case. We have:

$$U = \partial_x, \quad \beta = 1. \quad (2.15)$$

**Example 2.2.** The discrete case. The variable  $x$  is defined over an equally spaced lattice, with spacing  $\sigma$ . Two of the most common choices for the discrete derivative are:

a) The right discrete derivative.

$$U = \Delta^+ = \frac{T - 1}{\sigma}, \quad \beta = T^{-1}. \quad (2.16)$$

b) The left discrete derivative.

$$U = \Delta^- = \frac{1 - T^{-1}}{\sigma}, \quad \beta = T. \quad (2.17)$$

Other cases will be considered below.

Using the  $*$  multiplication of eq. (2.9) it is easy to construct the basic sequence for the operator  $U$ . Let us introduce the polynomial sequence of operators

$$P_n = (x\beta)^n, \quad n \in \mathbb{N}. \quad (2.18)$$

The delta operator  $U$  satisfies the relation

$$[U, (x\beta)^n] = n(x\beta)^{n-1}, \quad n \in \mathbb{N}. \quad (2.19)$$

This is an immediate consequence of the definition (2.13) and of the Leibnitz rule (2.11). A proof is obtained by induction. From (2.19) we immediately obtain:

$$U * P_n = nP_{n-1}, \quad n \in \mathbb{N} \quad (2.20)$$

This shows that  $\{(x\beta)^n\}_{n \in \mathbb{N}}$  is the basic sequence for the operator  $U$ , under the  $*$  multiplication.

**Definition 2.5** An umbral correspondence is a map  $\mathcal{R} : \mathcal{L} \rightarrow \mathcal{L}$  defined by

$$(x\beta_1)^n \xrightarrow{\mathcal{R}} (x\beta_2)^n, \quad (2.21)$$

where  $P_n^1 = \{(x\beta_1)^n\}$  and  $P_n^2 = \{(x\beta_2)^n\}$  are basic sequences of operators for two delta operators  $U_1$  and  $U_2$  respectively.

The umbral correspondence (2.21) naturally induces a correspondence between the two operators  $U_1$  and  $U_2$ , according to the following scheme:

$$\begin{array}{ccc} (x\beta_1)^n & \xleftrightarrow{\mathcal{R}} & (x\beta_2)^n \\ \mathfrak{I} \downarrow & & \mathfrak{I} \uparrow \\ U_1 & \xleftrightarrow{\mathcal{R}} & U_2. \end{array} \quad (2.22)$$

We shall also denote the induced correspondence between delta operators by the symbol  $\mathcal{R}$ .

Systems of equations connected by the umbral map (2.21) share many algebraic properties. A particular case of the umbral correspondence is when  $U_1$  is the standard derivative  $\partial_x$ , and  $U_2$  is a discrete derivative  $\Delta$ . Then according to the scheme (2.22) we have

$$\begin{array}{ccc} x^n & \xleftrightarrow{\mathcal{R}} & (x\beta)^n \\ \mathfrak{I} \downarrow & & \mathfrak{I} \uparrow \\ \partial_x & \xleftrightarrow{\mathcal{R}} & \Delta \end{array} \quad (2.23)$$

Let us observe that Definition 2.5 generalizes the notion of an umbral operator introduced in [13]: an umbral operator  $R : \mathcal{P} \rightarrow \mathcal{P}$  is an operator (in general not necessarily shift-invariant) which maps some basic sequence of polynomials  $p_n(x)$  into another basic sequence  $q_n(x)$ :

$$p_n(x) \xleftrightarrow{R} q_n(x). \quad (2.25)$$

Indeed, we observe that, since  $\beta$  is a function of shifts and any constant is invariant under the action of a shift operator, an umbral operator  $R$  is deduced from the action of  $\mathcal{R}$  simply applying the sequence of operators  $(x\beta)^n$  onto 1:

$$(x\beta_1)^n \cdot 1 \xleftrightarrow{R} (x\beta_2)^n \cdot 1. \quad (2.26)$$

From (2.19) we also get

$$U_i (x\beta_i)^n \cdot 1 = n (x\beta_i)^{n-1} \cdot 1, \quad i = 1, 2. \quad (2.27)$$

An important consequence is that the umbral correspondence (2.22) preserves commutation relations between operators in  $\mathcal{L}$ . In particular, it preserves Lie algebras.

Indeed, let  $A_1$  be a  $m$ -dimensional Lie algebra, generated by vector fields  $\{\mathbf{v}_i\}_{i=1,\dots,m}$  of the form

$$\mathbf{v}_i = \sum_j a_j (x_1, \dots, x_p) \partial_{x_j}. \quad (2.28)$$

The umbral correspondence (2.22) maps  $A_1$  isomorphically into an algebra  $A_2$ , generated by the vector fields  $\{\mathbf{v}_i^U\}_{i=1,\dots,m}$ , with

$$\mathbf{v}_i^U = \sum_j a_j (x_1 \beta_{x_1}, \dots, x_p \beta_{x_p}) \Delta_{x_j}. \quad (2.29)$$

This follows from the fact that the umbral correspondence (2.22) preserves the Heisenberg–Weyl algebra.

## 2.2 Umbral Calculus and Linear Difference Operators

The umbral approach reveals its power in the study of linear difference operators.

For our purposes, namely the study of difference equations and their continuous limits, we shall need only two types of delta operators. The first is simply the derivative  $U = \partial_x$ , with  $\beta = 1$ . The second is a general difference operator that has  $\partial_x$  as its continuous limit. We put

$$U \equiv \Delta = \frac{1}{\sigma} \sum_{k=l}^m a_k T_\sigma^k, \quad l, m \in \mathbb{Z}, \quad l < m \quad (2.30)$$

where  $a_k$  and  $\sigma$  are constants and  $T_\sigma \equiv T$  is the shift operator of eq.(2.4). In order for  $\Delta$  in (2.30) to be a delta operator, it must satisfy eq.(2.5). For any function  $f(x) \in \mathfrak{F}$  eq. (2.30) implies

$$\Delta f(x) = \frac{1}{\sigma} \sum_{k=l}^m a_k T^k f(x) = \frac{1}{\sigma} \sum_{k=l}^m a_k f(x + k\sigma). \quad (2.31)$$

Using a Taylor expansion around  $\sigma = 0$  we get

$$\Delta f(x) = \frac{1}{\sigma} \sum_{q=0}^{\infty} \frac{f^{(q)}(x)}{q!} \sigma^q \sum_{k=l}^m a_k k^q \quad (2.32)$$

Choosing  $f(x) = x$  we immediately see that eq. (2.5) implies

$$\sum_{k=l}^m a_k = 0, \quad (2.33)$$

and  $\sum_{k=l}^m a_k k = c$ . We require that in the continuous limit  $\Delta$  be the derivative  $\partial_x$ ; this implies  $c = 1$ , i.e.

$$\sum_{k=l}^m a_k k = 1. \quad (2.34)$$

Eq. (2.30) involves  $m - l + 1$  constants  $a_k$ , subject to two conditions (2.33) and (2.34). To fix all constants  $a_k$  we must impose  $m - l - 1$  further conditions, for instance

$$\gamma_q \equiv \sum_{k=l}^m a_k k^q = 0, \quad q = 2, 3, \dots, m - l. \quad (2.35)$$

Conditions (2.33) and (2.34) are necessary and sufficient for  $U = \Delta$  to be a delta operator which has the derivative  $\partial_x$  as its continuous limit.

**Definition 2.6** *A difference operator of order  $p = m - l$  is a delta operator of the form (2.30) satisfying eqs. (2.33) and (2.34).*

**Theorem 2.1** *If the difference operator  $\Delta$  of order  $(m - l) \geq 2$  satisfies the supplementary conditions (2.35) it provides an approximation of order  $\sigma^{m-l}$  of the derivative  $\partial_x$ .*

**Proof.** We immediately have from eq. (2.32) and eqs. (2.33), (2.34) and (2.35)

$$\Delta f \underset{\sigma \rightarrow 0}{\sim} f'(x) + \frac{\sigma^{m-l}}{(m-l+1)!} f^{(m-l-1)}(x) \sum_{k=l}^m a_k k^{m-l-1}. \quad (2.36)$$

**QED**

**Remark.** Formula (2.30) defines  $U$  as an operator parametrized by  $\sigma$ , where  $\sigma \in \mathbb{F}$ . It may happen that for specific values of  $\sigma$  the operator  $U$  could involve less than  $p$  points, and consequently its order would be less than  $p$ . Once a representation of  $U$  as a difference operator is chosen, these points can be easily determined by solving a linear system of algebraic equations.

By way of an example, let us consider the following equation [40]:

$$\Delta^3 f(x) + 3\Delta^2 f(x) + \Delta f(x) - f(x) = 0. \quad (2.37)$$

If  $\Delta = \frac{T-1}{\sigma}$ , for  $\sigma = 1$  eq. (2.37) becomes

$$f(x+3) - f(x+1) = 0,$$

which is of second order, in an appropriate domain.

In the following,  $U$  will be assumed to be an operator of order  $p$  parametrically depending on  $\sigma$ , and we shall omit the simple analysis of the specific cases in which the order could be less than maximal.

**Theorem 2.2** *If  $\Delta$  is a difference operator of order  $p$ , then  $\tilde{\Delta} = T^j \Delta$ ,  $j \in \mathbb{Z}$  is a difference operator of the same order.*

**Proof.** Let us first prove the result for  $j = 1$ . We have

$$T\Delta = \frac{1}{\sigma} \sum_{k=l}^m a_k T^{k+1} = \frac{1}{\sigma} \sum_{k=l-1}^{m+1} \tilde{a}_k T^k, \quad \tilde{a}_k = a_{k-1}.$$

Hence

$$\begin{aligned} \sum_{k=l+1}^{m+1} \tilde{a}_k &= \sum_{k=l}^m a_k = 0 \\ \sum_{k=l+1}^{m+1} k \tilde{a}_k &= \sum_{k=l}^m (k+1) a_k = \sum_{k=l}^m k a_k = 1. \end{aligned}$$

Thus, conditions (2.31) and (2.33) are satisfied for  $\tilde{U}$  and that is all that is needed. The proof for  $j = -1$  is analogous and for  $j$  arbitrary the result follows by induction. **QED**

Conditions (2.35) are not shift invariant. However, once  $m$  and  $l$  are chosen equations (2.35) can always be imposed. Their solution depends on  $m$  and  $l$ , not only on the shift invariant difference  $m - l$ .

**Theorem 2.3** *The operator  $\beta$  conjugate to the difference operator  $\Delta$  of eq. (2.30) is*

$$\beta = \left( \sum_{k=l}^m a_k k T^k \right)^{-1}. \quad (2.38)$$

**Proof.** Using eq. (2.14) we have

$$\beta = (\Delta')^{-1} = [\Delta, x]^{-1}.$$

Moreover

$$[\Delta, x] = \frac{1}{\sigma} \left( \sum_{k=l}^m a_k (x + k\sigma) T^k - x \sum_{k=l}^m a_k T^k \right) = \sum_{k=l}^m a_k k T^k$$

and (2.38) follows. **QED**

Examples of difference operators and the corresponding operators  $\beta$  are  $\Delta^+$  and  $\Delta^-$  of eq. (2.16) and (2.17). Both are of order 1. Higher order examples are

$$\Delta^s = \frac{T - T^{-1}}{2\sigma}, \quad \beta = \left( \frac{T + T^{-1}}{2} \right)^{-1}, \quad (2.39)$$

$$\Delta^{(III)} = -\frac{1}{6\sigma} (T^2 - 6T + 3 + 2T^{-1}), \quad \beta = \left( -\frac{T^2 - 3T - T^{-1}}{3} \right)^{-1} \quad (2.40)$$

$$\Delta^{(IV)} = -\frac{1}{12\sigma} (T^2 - 8T + 8T^{-1} - T^{-2}), \quad \beta = \left( -\frac{T^2 - 4T - 4T^{-1} + T^{-2}}{6} \right)^{-1}. \quad (2.41)$$

The operators  $\Delta^s$ ,  $\Delta^{(III)}$  and  $\Delta^{(IV)}$  approximate the derivative to order  $\sigma^2$ ,  $\sigma^3$  and  $\sigma^4$  respectively.

**Theorem 2.4** *The expression*

$$P_n(x) \equiv (x\beta)^n \cdot 1 \quad (2.42)$$

*is a well defined polynomial in  $x$  of order  $n$  with finite coefficients depending on a finite number of nonnegative powers of the shifts  $\sigma$  for any difference operator  $\Delta$ . The expression for  $P_n$  is*

$$P_n(x) = \sum_{k=1}^n A_k \sigma^{n-k} x^k, \quad A_n = 1, \quad (2.43)$$

where all coefficients  $A_k$  are finite and depend only on the coefficients  $a_k$  in the definition of  $\Delta$  (see eq. (2.30)). In particular, they do not depend on  $\sigma$ .

**Proof.** Let us consider the difference operator  $\Delta$  of eq. (2.30) and define the quantities

$$\gamma_j = \sum_{k=l}^m a_k k^j, \quad \gamma_0 = 0, \quad \gamma_1 = 1, \quad j = 0, 1, 2, \dots \quad (2.44)$$

Let us now prove eq. (2.43) by induction. Let  $P_n$  be a basic sequence of polynomials for any  $\Delta$ , as given by eq. (2.27). Thus we put

$$P_{n+1}(x) = \sum_{a=1}^{n+1} B_a x^a, \quad (2.45)$$

and must prove that the coefficients  $B_a$  are finite and depend on  $\sigma$  in the proper way (i.e.  $B_a = \tilde{B}_a \sigma^{n+1-a}$ , where  $\tilde{B}_a$  is finite and does not depend on  $\sigma$ ).

We rewrite eq. (2.27) (with  $n$  substituted by  $n+1$ ) as

$$\Delta P_{n+1} = (n+1) P_n. \quad (2.46)$$

The left hand side is

$$\begin{aligned} \Delta P_{n+1} &= \frac{1}{\sigma} \sum_{b=l}^m a_b \sum_{a=1}^{n+1} B_a (x + b\sigma)^a = \sum_{a=1}^{n+1} B_a \sum_{k=0}^a \binom{a}{k} x^k \sigma^{a-k-1} \gamma_{a-k} \\ &= \sum_{k=0}^{n+1} \sum_{a=k}^{n+1} B_a \binom{a}{k} x^k \sigma^{a-k-1} \gamma_{a-k}. \end{aligned}$$

Comparing powers on the left and right hand side of eq. (2.46), we obtain a system of linear algebraic equations for the coefficient  $B_k$ :

$$\sum_{a=k}^{n+1} B_a \binom{a}{k} \sigma^{a-k-1} \gamma_{a-k} = (n+1) A_k \sigma^{n-k}. \quad (2.47)$$

The system (2.47) has a triangular structure. For  $k = n+1$ , we get the identity  $0 = 0$ . For  $k = n$ , only one term is present on the left and we get  $B_{n+1} = 1$  (since we have  $\gamma_0 = 0$  and  $A_n = 1$ ). The value  $k = n-1$  gives

$$B_n = \sigma \frac{n+1}{n} \left( A_{n-1} - \frac{n}{2} \right).$$

In general, the system (2.47) implies

$$B_{n-j} = \sigma^{j+1} \sum_{k=n-j-1}^n \mu_k A_k \quad (2.48)$$

where the coefficients  $\mu_k$  are easy to calculate, but are cumbersome (and of little interest), so we do not spell them out. **QED**

Let us present the first few basic polynomials  $P_k(x) = (x\beta)^k 1$  for arbitrary  $\Delta$  as given by eq. (2.30) with  $\gamma_j$  defined in terms of  $a_k$  by eq. (2.44). We obtain

$$\begin{aligned} P_0 &= (x\beta)^0 \cdot 1 = 1 \\ P_1 &= (x\beta)^1 \cdot 1 = x \\ P_2 &= (x\beta)^2 \cdot 1 = x^2 - \sigma\gamma_2 x \\ P_3 &= (x\beta)^3 \cdot 1 = x^3 - 3\sigma\gamma_2 x^2 - \sigma^2 (\gamma_3 - 3\gamma_2^2) x \\ P_4 &= (x\beta)^4 \cdot 1 = x^4 - 6\sigma\gamma_2 x^3 + \sigma^2 (-4\gamma_3 + 15\gamma_2^2) x^2 \\ &\quad + \sigma^3 (-\gamma_4 + 10\gamma_2\gamma_3 - 15\gamma_2^3) x. \end{aligned} \quad (2.49)$$

For  $\sigma \rightarrow 0$ , we obviously reobtain the basic series (sequence) for  $\Delta = \partial_x$ .

For  $\Delta^+ = \frac{T-1}{\sigma}$  we have only two values of  $a_j$ , namely  $a_1 = 1$ ,  $a_0 = -1$ , hence  $\gamma_j = 1$ ,  $j = 2, 3, \dots$ . The polynomials (2.49) in this case reduce to the well-known factorial powers  $P_n = x(x-\sigma)(x-2\sigma)\dots(x-(n-1)\sigma)$ .

### 2.3 Linear Difference Equations and Umbral Equations

Let us introduce the notation  $\hat{f} = f(x\beta)$ , i.e. to each function  $f(x) \in \mathfrak{F}$  we associate an operator  $\hat{f} \in \mathfrak{L}$ . We shall consider an operator equation of the form

$$\sum_{k=0}^n \hat{A}_k U^k \hat{f} = \hat{g} \quad (2.50)$$

where  $U$  is a delta operator and  $\beta$  is its conjugate operator defined in eqs. (2.13)–(2.14). We assume that the operators  $\hat{A}_k$  and  $\hat{g}$  can be expanded into formal power series in  $(x\beta)$ .

**Definition 2.7** *An umbral equation of order n is an operator equation of the form (2.50) in which the operators  $\hat{A}_k$  and  $\hat{g}$  are given. The unknown is the operator  $\hat{f}$ .*

If  $U$  is specified to be  $U = \partial_x$ , then  $\beta = 1$  and eq. (2.50) reduces to a differential equation of order  $n$ . If  $U$  is a difference operator, (2.50) is still an operator equation. Projecting both sides onto a space of functions, i.e. applying them to a constant, we obtain a difference equation. The order of the difference equations obtained projecting eq. (2.50) may vary depending on the structure of the operator  $\widehat{A}_k$  (since it acts on the operator  $\widehat{f}$ ) and on the choice of the operator  $\Delta$  (and consequently of  $\beta$ ) in terms of shift operators.

Let us first take  $U = \partial_x$ ,  $\beta = 1$  in eq. (2.50). The obtained linear ODE will have  $n$  linearly independent solutions  $f_i(x)$ . We can expand them into formal power series about any point  $x_0$ , where  $x_0$  is not a singular point of the equation. Now let  $U = \Delta$  be a difference operator and  $\beta$  the corresponding conjugate operator. Then  $f_i(x\beta) \cdot 1$  viewed as a formal power series, will be a solution of the corresponding difference equation.

**Definition 2.8** *We shall call  $\widehat{f} \cdot 1$  an **umbral solution** of the difference equation*

$$\sum_{k=0}^n \widehat{A}_k U^k \widehat{f} \cdot 1 = \widehat{g} \cdot 1 \quad (2.51)$$

*if the real valued function  $f(x)$  is a solution of the differential equation*

$$\sum_{k=0}^n A_k \partial_x^k f(x) = g(x). \quad (2.52)$$

Thus each solution of the ODE (2.52) provides a formal power solution of the difference equation (2.51) (and of the umbral equation (2.50)). However, eq. (2.51) and (2.50) may have other solutions. Indeed, for a linear difference equation with constant coefficients we have the following theorem.

**Theorem 2.5** *Let  $U$  be a difference operator of order  $p$  and let us assume that the operators  $\widehat{A}_k$  in eq. (2.50) are constant. Equation (2.51) will then have  $np$  linearly independent solutions,  $n$  of them umbral ones.*

**Proof.** Eq. (2.51) in this case is a difference equation involving  $np + 1$  different points. Hence to obtain a solution in a new point we must specify initial conditions in  $np$  points. This provides  $np$  linearly independent solutions, uniquely defined in the lattice points  $x_n = x_0 + n\sigma$  [40, 41]. Now, let us consider the continuous limit of eq. (2.51). It is a linear partial differential

equation of order  $n$ , possessing analytic solutions which can be expanded around any nonsingular point. Applying the umbral correspondence to the series expansion of these solutions, we obtain  $n$  solutions of eq. (2.51) which are expressed as formal power series in  $(x\beta)^k$ , and therefore are elements of the algebra  $\mathfrak{F}$ . These are the umbral solutions admitted by eq. (2.51). The remaining  $(n - 1)p$  do not belong to  $\mathfrak{F}$ . **QED**

When  $A_k$  are polynomials in  $(x\beta)$ , then additional shifts may appear in the explicit form of the equations coming from the umbral equation (2.50) via projection and their order may be different than  $np$ .

As an example, let us consider the "umbral Airy equation"

$$[\Delta^2 + ax\beta] \widehat{\Psi} = 0, \quad a = \text{const.} \quad (2.53)$$

For  $\Delta^+ = (T - 1)/\sigma$ ,  $\beta = T^{-1}$  and  $\tilde{\Psi}(x) = \widehat{\Psi} \cdot 1$  we have

$$\frac{1}{\sigma^2} [\tilde{\Psi}(x + 2\sigma) - 2\tilde{\Psi}(x + \sigma) + \tilde{\Psi}(x)] + ax\tilde{\Psi}(x - \sigma) = 0.$$

This is a third order difference equation since it involves the function  $\tilde{\Psi}(x)$  at the points  $x + 2\sigma$ ,  $x + \sigma$ ,  $x$  and  $x - \sigma$ . For  $\Delta = \Delta^s$  eq. (2.53) would seem to involve infinitely many points:

$$\frac{1}{4\sigma^2} [\tilde{\Psi}(x + 2\sigma) - 2\tilde{\Psi}(x) + \tilde{\Psi}(x - 2\sigma)] + ax \left( \frac{T + T^{-1}}{2} \right)^{-1} \tilde{\Psi}(x) = 0. \quad (2.54)$$

However, multiplying eq. (2.54) by  $\beta^{-1}$  we obtain

$$\frac{1}{4\sigma^2} [\tilde{\Psi}(x + 3\sigma) - \tilde{\Psi}(x + \sigma) - \tilde{\Psi}(x - \sigma) + \tilde{\Psi}(x - 3\sigma)] + ax\tilde{\Psi}(x) = 0 \quad (2.55)$$

This equation is a 6th order difference equation.

As a simple example of umbral and nonumbral solutions, let us consider a first order homogeneous umbral equation with constant coefficients:

$$U\widehat{f} = a\widehat{f}, \quad a \neq 0. \quad (2.56)$$

For  $U = \partial_x$ , the solution is

$$f(x) = Ae^{ax}. \quad (2.57)$$

Now, let us consider the first order difference operator  $\Delta^+$ . Eq. (2.56) reduces to

$$f(x + \sigma) - f(x) = a\sigma f(x). \quad (2.58)$$

We look for a solution in the form  $f(x) = \lambda^x$  and find

$$\lambda = (1 + a\sigma)^{\frac{1}{\sigma}}. \quad (2.59)$$

Thus we obtain a single solution

$$f_1(x) = A(1 + a\sigma)^{\frac{x}{\sigma}} \quad (2.60)$$

and of course we have

$$\lim_{\sigma \rightarrow 0} f(x) = Ae^{ax}. \quad (2.61)$$

The umbral correspondence provides the solution

$$f_u(x) = Ae^{axT^{-1}} \cdot 1. \quad (2.62)$$

Expanding (2.60) and (2.62) in formal power series in  $a$ , we find that the two series coincide, i.e.  $f_1 = f_u$ .

For comparison, let us consider the second order difference operator  $\Delta^s$ . Equation (2.56) in this case yields

$$f(x + \sigma) - f(x - \sigma) = 2\sigma a f(x). \quad (2.63)$$

Putting  $f(x) = \lambda^x$  we obtain two values of  $\lambda$  and the general solution of eq. (2.63) in this case is

$$f = A_1 \left( \sqrt{1 + a^2\sigma^2} + a\sigma \right)^{\frac{x}{\sigma}} + A_2 (-1)^{\frac{x}{\sigma}} \left( \sqrt{1 + a^2\sigma^2} - a\sigma \right)^{\frac{x}{\sigma}} = A_1 f_1 + A_2 f_2. \quad (2.64)$$

The first solution has  $e^{ax}$  as its continuous limit. The second one does not have a limit for  $\sigma \rightarrow 0$ . The umbral correspondence provides the solution

$$f_u(x) = A e^{ax \left( \frac{T+T^{-1}}{2} \right)^{-1}} \cdot 1 \quad (2.65)$$

(see eq. (2.39)). Expanding into formal power series in  $a$  we find  $f_u = f_1$  and  $f_2$  is nonumbral.

The question arises whether an expression of the type

$$\hat{f} = e^{ax\beta} \quad (2.66)$$

is meaningful, at least in the sense of a formal power series. The problem is that for a general difference operator  $\Delta$ , the expression for  $\beta$ , given in eq. (2.38), is quite complicated. If we expand  $\beta$  into a power series in  $T$ , it

will for  $m - l \geq 3$  involve infinitely many shifts. Convergence problems may arise. Luckily, it is not eq. (2.66) itself that provides the umbral solution of a difference equation. Rather, it is the projection of the operator  $\hat{f}$  onto a space of functions, or formal power series. The expressions that appear in the corresponding expansions are  $P_n(x) = (x\beta)^n \cdot 1$  and these are finite polynomials in  $x$ , and in the shifts  $\sigma$ , with well defined finite coefficients (see Theorem 2.4). As a matter of fact these are the basic polynomials for the difference operator  $\Delta$  defined in eq. (2.30).

It follows that if we know a solution of the umbral equation (2.50) for  $U = \partial_x$ , and have

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} x^n,$$

then for  $U = \Delta$  as in (2.30) the corresponding umbral solution will be

$$\hat{f} \cdot 1 = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} P_n(x).$$

The matter of convergence is a separate issue.

Umbral calculus and specially the umbral correspondence also provide us with a powerful tool with which to handle symmetries of linear difference equations, both ordinary and partial ones. On one hand, we can discretize a linear differential equation, in particular the linear Schrödinger equation, via the (multidimensional) umbral substitutions

$$\partial_{x_i} \xrightarrow{\mathcal{R}} \Delta_{x_i}, \quad x_i \xrightarrow{\mathcal{R}} x_i \beta_{x_i}, \quad \partial_t \xrightarrow{\mathcal{R}} \Delta_t, \quad t \xrightarrow{\mathcal{R}} t \beta_t.$$

Lie symmetries, both point and generalized ones, of linear differential equations can be expressed in terms of commuting operators. Since the umbral correspondence preserves commutation relations, it will also preserve symmetries. However, we may have more symmetries than in the continuous case due to the nonumbral solutions of the determining equations.

### 3 Discretization of the Time Dependent Schrödinger Equation Preserving all Point Symmetries

Before considering discrete space-time, let us first give a detailed and rigorous analysis of the point symmetries of the time-dependent Schrödinger equation in continuous space-time. The results will be presented in a form well suited for the discretization.

### 3.1 Point Symmetries and Commuting Operators in Continuous Space-Time

We write the Schrödinger equation in  $\mathbb{R}^{n+1}$  as

$$L\psi = 0, \quad L = i\partial_t - H, \quad H = -\frac{1}{2}\sum_{k=1}^n \frac{\partial^2}{\partial x_k^2} + V(\vec{x}, t). \quad (3.1)$$

A local Lie point symmetry transformation is generated by a vector field that we write in evolutionary form [42] as

$$\mathbf{v}^E = Q\partial_\psi + Q^*\partial_{\psi^*}, \quad (3.2)$$

$$Q = \eta - \tau \frac{\partial \psi}{\partial t} - \xi_k \frac{\partial \psi}{\partial x_k}. \quad (3.3)$$

The functions  $\eta, \tau$  and  $\xi_k$  depend on  $t, \vec{x}, \psi$  and  $\psi^*$  where the star denotes complex conjugation. These functions are determined from the requirement

$$pr^{(2)}\mathbf{v}^E(L\psi)|_{L\psi=L^*\psi^*=0}=0, \quad pr^{(2)}\mathbf{v}^E(L^*\psi^*)|_{L\psi=L^*\psi^*=0}=0. \quad (3.4)$$

The following theorem will provide a basis for studying the symmetries of a nonrelativistic quantum system.

**Theorem 3.1** *All Lie point symmetries of the time-dependent Schrödinger equation (3.1) are generated by evolutionary vector fields of the form (3.2) with*

$$Q = \chi(\vec{x}, t) + iX\psi, \quad (3.5)$$

$$X = i(\tau(t)\partial_t + \xi_k(\vec{x}, t)\partial_{x_k} - i\phi(\vec{x}, t)), \quad (3.6)$$

$$\xi_k(\vec{x}, t) = \frac{1}{2}x_k\tau' - A_{kl}x_l + f_k(t), \quad (3.7)$$

$$\phi(\vec{x}, t) = \frac{1}{4}\tau''r^2 + x_kf'_k + g(t) + i\left[\frac{n}{4}\tau' - B\right], \quad (3.8)$$

where the prime denotes a derivative. The function  $\chi(\vec{x}, t)$  satisfies the Schrödinger equation (3.1),  $A_{kl} = -A_{lk}$  and  $B$  are real constants. The real functions  $\tau(t)$ ,  $f_k(t)$ ,  $g(t)$  and the constants  $A_{kl}$  depend on the potential and satisfy the equation

$$\tau(t)V_t + \xi_k(\vec{x}, t)V_{x_k} + \tau'V + \frac{1}{4}\tau'''r^2 + x_kf''_k + g' = 0, \quad (3.9)$$

with  $r^2 = \sum_{k=1}^n x_k^2$ . Moreover, the linear operator  $X$  commutes with  $L$  on the solutions of the Schrödinger equation

$$[L, X] \psi |_{L\psi=0} = 0. \quad (3.10)$$

**Proof.** Eq. (3.4) implies a system of determining equations. Those among them that come from terms involving derivatives of  $\psi$ , e.g.  $\psi_x \psi_{xx}$ ,  $\psi_{xx}$ ,  $\psi_x^k$ ,  $k \geq 1$  do not depend on the potential  $V(\vec{x}, t)$ . From them we obtain the fact that the corresponding transformations are fiber preserving and linear (inhomogeneous). That is,  $Q$  has the form (3.3) with  $\tau$  and  $\xi_k$  independent of  $\psi$  and  $\psi^*$ . From the same equations we find that  $\tau$  depends only on  $t$  and that  $\xi_k(\vec{x}, t)$  are linear in  $\vec{x}$ . Thus  $\xi_k$  and  $\phi$  have the form (3.7) and (3.8), respectively.

Once these conditions are satisfied, only one determining equation remains, namely eq. (3.9), involving the potential in a crucial manner.

To prove the commutativity relation (3.10) we use the compatibility of the two flows

$$i \frac{\partial \psi}{\partial t} = H\psi, \quad \frac{\partial \psi}{\partial \lambda} = Q, \quad (3.11)$$

where  $\lambda$  is a group parameter and  $Q$  is the characteristic of the vector field (see eqs. (3.5)–(3.8)). Equating the cross derivatives  $\psi_{t\lambda} = \psi_{\lambda t}$  and using the equation  $L\chi(\vec{x}, t) = 0$ , we obtain

$$[H, X] \psi = -iX_t \psi, \quad (3.12)$$

where  $\psi$  is any solution of the Schrödinger equation. This is equivalent to eq. (3.10). Simply stated: finding point symmetries of the Schrödinger equation is equivalent to finding linear selfadjoint operators  $X$  commuting with  $L$  on the solution set of  $L$ . **QED**

### Comments.

1. For any potential  $V_k(\vec{x}, t)$  the function  $\chi(\vec{x}, t)$ , the constant  $B$  and a constant  $g = g_0$  are solutions of eq. (3.9). Hence we always have a "trivial" symmetry algebra

$$\begin{aligned} S(\chi) &= \chi(\vec{x}, t) \partial_\psi + \chi^*(\vec{x}, t) \partial_{\psi^*}, & L\chi &= 0 \\ N &= \psi \partial_\psi + \psi^* \partial_{\psi^*} & (3.13) \\ E &= i(\psi \partial_\psi - \psi^* \partial_{\psi^*}), \end{aligned}$$

due to the linearity of the Schrödinger equation.

2. Each symmetry generator  $\mathbf{v}^E$  provides us with a flow that is by construction compatible with the time flow (3.1), that is, we can simultaneously solve the equations (3.11). The fixed point  $\partial\psi/\partial\lambda = 0$  corresponds to group invariant solutions.
3. While the result presented in Theorem (3.1) is quite simple and natural, we have not found it explicitly in the literature, so we have sketched a proof. For other results on point symmetries of linear differential equations, see. e.g. [43], [44] and [45].

Let us consider the implications of Theorem 3.1 for special cases of the potential  $V(\vec{x}, t)$ . We shall omit the operators (3.13) that are present for any potential  $V(\vec{x}, t)$ .

Let us first consider the free Schrödinger equation (for further discussions, see also [46]). For  $V(\vec{x}, t) = 0$  in  $\mathbb{R}^{3+1}$  the so called "Schrödinger group" was first obtained by Niederer [47]. For  $n$  arbitrary we obtain its generalization, i.e. the group  $Sch(n)$ . Its Lie algebra can be written as

$$\begin{aligned} P_0 &= \partial_t, \quad D = 2t\partial_t + x_k\partial_{x_k} - \frac{1}{2}(\psi\partial_\psi + \psi^*\partial_{\psi^*}), \\ C &= t^2\partial_t + tx_k\partial_{x_k} - \frac{1}{2}t(\psi\partial_\psi + \psi^*\partial_{\psi^*}) + \frac{in}{4}r^2(\psi\partial_\psi - \psi^*\partial_{\psi^*}), \\ L_{ik} &= x_i\partial_{x_k} - x_k\partial_{x_i}, \quad P_k = \partial_{x_k}, \\ B_k &= t\partial_{x_k} + \frac{i}{2}x_k(\psi\partial_\psi - \psi^*\partial_{\psi^*}), \\ E &= i(\psi\partial_\psi - \psi^*\partial_{\psi^*}). \end{aligned} \tag{3.14}$$

The Levi decomposition [48] of this algebra for  $n \geq 3$  is

$$\mathfrak{L} \sim [sl(2, \mathbb{R}) \oplus O(n)] \oplus H_n \tag{3.15}$$

where the radical  $H_n$  is the  $n$ -dimensional Heisenberg algebra. Explicitly we have

$$sl(2, \mathbb{R}) \sim \{P_0, D, C\}, \quad O(n) \sim \{L_{ik}\}, \quad H_n \sim \{P_k, B_k, E\}. \tag{3.16}$$

We included the central element  $E$  explicitly in (3.14) since it appears in the derived algebra of the Schrödinger algebra (it is also present in (3.13)).

Eq. (3.9) implies that for a general time independent potential  $V(\vec{x})$  we have only one additional symmetry generator to the set given by eqs. (3.13), namely time translations  $P_0 = \partial_t$ .

For a central potential  $V = V(r)$ , the additional elements are time translations and rotations

$$P_0 = \partial_t, \quad L_{ik} = x_i \partial_{x_k} - x_k \partial_{x_i}, \quad 1 \leq i \leq k \leq n. \quad (3.17)$$

In the case of a translationally invariant potential  $V = V(x_n)$ , the additional symmetry elements are

$$\begin{aligned} P_0 &= \partial_t, P_j = \partial_{x_j}, B_j = t \partial_{x_j} - ix_j (\psi \partial_\psi - \psi^* \partial_{\psi^*}), \quad 1 \leq j \leq n-1, \\ L_{ik} &= x_i \partial_{x_k} - x_k \partial_{x_i}, \quad 1 \leq i \leq k \leq n-1. \end{aligned} \quad (3.18)$$

### 3.2 Symmetries of the discrete time dependent Schrödinger equation

The umbral correspondence, together with Theorem 3.1 provide the tools necessary for a symmetry preserving discretization of quantum mechanics.

Indeed, let us consider a discrete space-time, more precisely an  $n+1$  dimensional orthogonal and equally spaced lattice with time step  $\sigma_t$  and space steps  $\sigma_k$ ,  $1 \leq k \leq n$ . In this space we write a "Schrödinger difference equation"

$$L_D \psi = 0, \quad L = i \Delta_t - H_D \quad (3.19)$$

$$H_D = -\frac{1}{2} \sum_{k=1}^n \Delta_{x_k x_k} + V(x_1 \beta_1, \dots, x_n \beta_n, t \beta_t)$$

where we have

$$[\Delta_{x_k}, x_k \beta_k] = 1, \quad [\Delta_t, t \beta_t] = 1. \quad (3.20)$$

Each  $\Delta_{x_k}$ ,  $\Delta_t$  is some chosen difference operator and  $\beta_k$ ,  $\beta_t$  are the corresponding conjugate operators satisfying the Heisenberg commutation relations (3.20).

The continuous limit of eq. (3.19) is eq. (3.1), obtained by taking  $\sigma_k \rightarrow 0$ ,  $\sigma_t \rightarrow 0$ , i.e.

$$\Delta_{x_k x_k} \rightarrow \frac{\partial^2}{\partial x_k^2}, \quad \Delta_t \rightarrow \partial_t, \quad \beta_i \rightarrow 1, \quad \beta_t \rightarrow 1. \quad (3.21)$$

Let us assume that in the continuous limit the obtained Schrödinger equation (3.1) is invariant under some Lie point symmetry group generated by some evolutionary vector field (3.2). Symmetries of linear difference equations on

fixed lattices can also be expressed in terms of evolutionary vector fields [28], [36]. For eq. (3.19) we put

$$\mathbf{v}_D^E = Q_D \partial_\psi + Q_D^* \partial_{\psi^*} \quad (3.22)$$

$$Q_D = \eta_D - \tau_D \Delta_t \psi - \xi_{k_D} \Delta_{x_k} \psi$$

where  $\eta_D$ ,  $\tau_D$  and  $\xi_{k_D}$  are functions of  $x_i \beta_i$ ,  $t \beta_t$ ,  $\psi$  and  $\psi^*$ . The functions  $\psi$  and  $\psi^*$  are to be evaluated at the points  $x_i \beta_i$ ,  $t \beta_t$ .

The prolongation of the vector field (3.22) must act on the dependent variables  $\psi$  and  $\psi^*$  and on their discrete derivatives  $\Delta_t \psi$ ,  $\Delta_{x_k x_k} \psi$ . As in the continuous case, we require that an infinitesimal transformation

$$\begin{aligned} \widetilde{x_k \beta_k} &= x_k \beta_k, & \widetilde{t \beta_t} &= t \beta_t \\ \widetilde{\psi}(\widetilde{x_k \beta_k}, \widetilde{t \beta_t}) &= \psi(x_k \beta_k, t \beta_t) + \lambda Q, & \lambda &\ll 1 \end{aligned} \quad (3.23)$$

should take a solution  $\psi$  into a solution  $\widetilde{\psi}$  of the same equation (in new variables). First of all, we have

$$\widetilde{\beta_k} = \beta_k, \quad \widetilde{\beta_t} = \beta_t \quad (3.24)$$

since  $\beta_k$  and  $\beta_t$  are expressed in terms of shifts operators and we are considering equations on a fixed (not transforming) lattice. Eq. (3.23) is an infinitesimal transformation in the evolutionary formalism, hence only the dependent variables transform. The transformation of the discrete derivatives is given by

$$\begin{aligned} \Delta_t \widetilde{\psi} &= \Delta_t \psi + \lambda \Delta_t Q \\ \Delta_{x_k x_k} \widetilde{\psi} &= \Delta_{x_k x_k} \psi + \lambda \Delta_{x_k x_k} Q \end{aligned} \quad (3.25)$$

where  $\Delta_t$ ,  $\Delta_{x_k}$ , etc. are discrete total derivatives. One can of course also introduce discrete partial derivatives [36], but we shall not need them here.

In terms of the vector fields  $\mathbf{v}_D^E$  of eq. (3.22) the prolongation of  $\mathbf{v}_D^E$  is

$$pr \mathbf{v}_D^E = Q_D \partial_\psi + Q_D^t \partial_{\Delta_t \psi} + Q_D^{x_k x_k} \partial_{\Delta_{x_k x_k} \psi} + \dots + c.c. \quad (3.26)$$

where *c.c.* denotes the complex conjugate terms and we have

$$Q_D^t = \Delta_t Q_D, \quad Q_D^{x_k x_k} = \Delta_{x_k x_k} Q_D. \quad (3.27)$$

The determining equations for the characteristic  $Q_D$  are obtained as in the continuous case, i.e. from the invariance condition

$$pr \mathbf{v}_D^E (L_D \psi) |_{L_D \psi = L_D^* \psi^* = 0} = 0, \quad pr \mathbf{v}_D^E (L_D^* \psi^*) |_{L_D \psi = L_D^* \psi^* = 0} = 0. \quad (3.28)$$

From this we conclude that the following theorem holds.

**Theorem 3.2** *The discrete time-dependent Schrödinger equation (3.19) allows a Lie algebra of "umbral symmetries" isomorphic to that of its continuous limit (3.1). This Lie algebra is realized by vector fields (3.22) with*

$$Q_D = \chi(x_k\beta_k, t\beta_t) + iX_D\psi \quad (3.29)$$

$$X_D = i \left[ \tau(t\beta_t) \Delta_t + \sum_k \xi_k \Delta_{x_k} - i\phi \right] \quad (3.30)$$

$$\xi_k = \frac{1}{2} x_k \beta_k \Delta_t \tau - \sum_{l=1}^n A_{kl} x_l \beta_l + f_k(t\beta_t) \quad (3.31)$$

$$\phi = \left[ \frac{1}{4} \Delta_{tt} \tau \sum_{k=1}^n (x_k \beta_k)^2 + \sum_{k=1}^n x_k \beta_k \Delta_t f_k + g(t\beta_t) \right] + i \left[ \frac{n}{4} (\Delta_t \tau) - B \right] \quad (3.32)$$

The function  $\chi$  satisfies the discrete Schrödinger equation (3.19),  $A_{kl} = -A_{lk}$  and  $B$  are real constants. The real functions  $\tau$ ,  $f_k$  and  $g$  all depend only on  $t\beta_t$  and the potential  $V(x_k\beta_k, t\beta_t)$  satisfies:

$$\tau \Delta_t V + \sum_{k=1}^n \xi_k \Delta_{x_k} V + (\Delta_t \tau) V + \frac{1}{4} (\Delta_{ttt} \tau) \sum_{k=1}^n (x_k \beta_k)^2 + \sum_{k=1}^n x_k \beta_k \Delta_{tt} f_k + \Delta_t g = 0. \quad (3.33)$$

Finally, the difference operator  $X_D$  commutes with  $L_D$  on the solutions of the discrete Schrödinger equation (3.19):

$$[L_D, X_D] \psi |_{L_D \psi = 0} = 0. \quad (3.34)$$

**Proof.** The proof of Theorem 3.2 is quite analogous to that of Theorem 3.1 in the continuous case. To see the similarities and differences, let us restrict ourselves to the case  $n = 2$ .

The invariance condition (3.28) implies the following determining equations

$$\xi_{k,\psi} = \xi_{k,\psi^*} = \tau_\psi = \tau_{\psi^*} = 0, \quad \Delta_{x_i} \tau = 0, \quad \phi_{\psi^*} = 0, \quad \phi_{\psi\psi} = 0, \quad (3.35)$$

$$\Delta_{x_1} \xi_2 + \Delta_{x_2} \xi_1 = 0, \quad (3.36)$$

$$\Delta_t \tau - 2\Delta_{x_1} \xi_1 = 0, \quad \Delta_t \tau - 2\Delta_{x_2} \xi_2 = 0, \quad (3.37)$$

$$2i\Delta_t \xi_1 + 2\Delta_{x_1} \phi_{1\psi} + \Delta_{x_1 x_1} \xi_1 + \Delta_{x_2 x_2} \xi_1 = 0,$$

$$2i\Delta_t\xi_2 + 2\Delta_{x_2}\phi_{1\psi} + \Delta_{x_1x_1}\xi_2 + \Delta_{x_2x_2}\xi_2 = 0, \quad (3.38)$$

$$\begin{aligned} & 2\psi \{\tau\Delta_t V + \xi_1\Delta_{x_1}V + \xi_2\Delta_{x_2}V + V\Delta_t\tau + V\phi_\psi\} \\ & - 2V\phi + 2i\Delta_t\phi + \Delta_{x_1x_1}\phi + \Delta_{x_2x_2}\phi = 0. \end{aligned} \quad (3.39)$$

It is now obvious that eq. (3.30), (3.31) and (3.32) (for  $n = 2$ ) provide a solution to eq. (3.35), ..., (3.38) and that (3.39) reduces to eq. (3.33), once (3.35), ..., (3.38) are solved. Eq. (3.34) then follows in exactly the same manner as in the continuous case. **QED.**

### Comment.

There is an important difference between the continuous and the discrete case. In Theorem 3.1 we presented the most general solution of the determining equations. In Theorem 3.2 we presented a solution and added the requirement that the solution should have the correct continuous limit. Take for instance the function  $\tau$ . Equations (3.35) for any  $\Delta_t$ ,  $\Delta_x$  allow the solution  $\tau(t, \beta_t)$ , i.e. an arbitrary function of time  $t$  and the "shift" operator  $\beta_t$  independently. For first order operators  $\Delta^\pm$  (see Section 2), the function  $\tau$  will depend only on  $(t\beta_t)$ . This follows from the determining equations, and agrees with the result of umbral correspondence. Moreover, the result will have the correct continuous limit. Thus the discretization and the continuous equation have isomorphic symmetry algebras. For other choices of the discrete derivatives we may get more general solutions. For instance, let us consider the case of a "symmetric" derivative:

$$\Delta_x^s\tau = \frac{T_x - T_x^{-1}}{2\sigma}\tau = \frac{\tau(x + \sigma) - \tau(x - \sigma)}{2\sigma} = 0. \quad (3.40)$$

Eq. (3.40) has the general solution

$$\tau = \tau_0(t) + \tau_1(t)e^{\frac{i\pi x}{\sigma}}, \quad (3.41)$$

$$x = x_n = x_0 + n\sigma. \quad (3.42)$$

We see that eq. (3.40) actually allows an  $x$ -dependence in  $\tau$ . However, the second term in (3.42) does not have a continuous limit (for  $\sigma = x_{n+1} - x_n \rightarrow 0$ ).

### 3.3 Examples

As in the continuous case, for any discrete potential we have the "trivial" symmetries (3.13) (with  $\vec{x}$ ,  $t$  replaced by  $x_k\beta_k$ ,  $t\beta_t$ ).

Let us consider the case  $V = 0$ , i.e. a free quantum particle in discrete space time of dimension  $n + 1$ . Operators commuting with the operator  $L$  of eq. (3.19) are obtained from (3.14) by the umbral correspondence. We obtain the "discrete" Schrödinger algebra

$$\begin{aligned} P_0 &= \Delta_t, & D &= 2(t\beta_t)\Delta_t + \sum_{k=1}^n (x_k\beta_k)\Delta_{x_k} - \frac{1}{2}(\psi\partial_\psi + \psi^*\partial_{\psi^*}) \\ C &= (t\beta_t)^2\Delta_t + \sum_{k=1}^n (t\beta_t)(x_k\beta_k)\Delta_{x_k} - \frac{1}{2}(t\beta_t)(\psi\partial_\psi + \psi^*\partial_{\psi^*}) + \\ &\quad \frac{in}{4}\sum_{k=1}^n (x_k\beta_k)^2(\psi\partial_\psi - \psi^*\partial_{\psi^*}) \\ L_{ik} &= (x_i\beta_i)\Delta_{x_k} - (x_k\beta_k)\Delta_{x_i}, & P_k &= \Delta_{x_k}, \\ B_k &= (t\beta_t)\Delta_{x_k} + \frac{i}{2}(x_k\beta_k)(\psi\partial_\psi - \psi^*\partial_{\psi^*}) \\ E &= i(\psi\partial_\psi - \psi^*\partial_{\psi^*}). \end{aligned} \tag{3.43}$$

For a general time independent potential  $V(x_i\beta_i)$  we have only one additional (to (3.13)) symmetry generator, namely time translations  $P_0 = \Delta_t$ .

For a time independent central potential  $V = V\left(\sum_i (x_i\beta_i)^2\right)$  the additional symmetries are expressed by the operators

$$P_0 = \Delta_t, \quad L_{ik} = x_i\beta_i\Delta_{x_k} - x_k\beta_k\Delta_{x_i}, \quad 1 \leq i \leq k \leq n. \tag{3.44}$$

For a translationally invariant potential  $V = V(x_n\beta_n)$  the additional symmetry operators are

$$\begin{aligned} P_0 &= \Delta_t, \\ P_j &= \Delta_{x_j}, \quad B_j = t\beta_t\Delta_{x_j} - ix_j\beta_j(\psi\Delta_\psi - \psi^*\Delta_{\psi^*}), \quad 1 \leq j \leq n-1 \\ L_{ik} &= x_i\beta_i\Delta_{x_k} - x_k\beta_k\Delta_{x_i}, \quad 1 \leq i \leq k \leq n-1. \end{aligned} \tag{3.45}$$

## 4 Discrete Superintegrable Systems

The umbral calculus provides a systematic method for transferring results from standard quantum mechanics to quantum mechanics in a discrete space-time. This is particularly simple if the results are formulated in terms of commuting differential operators. It has been shown elsewhere [5] that there is a direct relation between generalized symmetries in quantum mechanics and higher order differential operators, commuting with the Hamiltonian. Here we shall briefly sum up the results and then adapt them to the discrete case.

### 4.1 Generalized Symmetries in Quantum Mechanics

Let us consider the stationary Schrödinger equation in real two-dimensional Euclidean space

$$H\psi = E\psi, \quad H = -\frac{1}{2}\Delta + V(x, y), \quad (4.1)$$

and look for second order generalized symmetries in their evolutionary form  $\mathbf{v}^E$  (3.2) with characteristic  $Q$  satisfying

$$Q = Q(x, y, \psi, \psi_x, \psi_y, \psi_{xx}, \psi_{xy}, \psi_{yy}). \quad (4.2)$$

We require that the second prolongation of the vector field  $\mathbf{v}^E$  should annihilate eq. (4.1) on its solution space, i.e.

$$\begin{aligned} pr^{(2)}\mathbf{v}^E(H - E)\psi &|_{\substack{H\psi=E\psi \\ H\psi^*=E\psi^*}} = 0, & pr^{(2)}\mathbf{v}^E(H - E)\psi &|_{\substack{H\psi=E\psi \\ H\psi^*=E\psi^*}} = 0. \end{aligned} \quad (4.3)$$

If we also require that  $Q$  be energy independent, we obtain the following result.

**Theorem 4.1** *The characteristic  $Q$  of the evolutionary vector field  $\mathbf{v}^E = Q\partial_\psi + Q^*\partial_{\psi^*}$ , corresponding to a second order generalized symmetry of the Schrödinger equation (4.1) has the form*

$$Q = X\psi + \chi(x, y) \quad (4.4)$$

$$\begin{aligned} X = & aL_3^2 + b(L_3P_1 + P_1L_3) + c(L_3P_2 + P_2L_3) + d(P_1^2 - P_2^2) \quad (4.5) \\ & + 2eP_1P_2 + \alpha L_3 + \beta P_1 + \gamma P_2 + \phi(x, y). \end{aligned}$$

The function  $\chi(x, y)$  satisfies the Schrödinger equation (4.1). The operator  $X$  commutes with the Hamiltonian  $H$

$$[H, X] = 0. \quad (4.6)$$

The quantities  $a, \dots, e, \alpha, \beta, \gamma$  are constants and

$$P_1 = \partial_x, \quad P_2 = \partial_y, \quad L_3 = y\partial_x - x\partial_y \quad (4.7)$$

are generators of the Euclidean group  $E_2$ .

For a proof of Theorem 4.1, see Ref. [5].

The commutativity relation (4.6) is equivalent to the following linear partial differential equations satisfied by the potential  $V(x, y)$  and the function  $\phi(x, y)$

$$[\alpha(y\partial_x - x\partial_y) + \beta\partial_x + \gamma\partial_y] V(x, y) = 0, \quad (4.8)$$

$$\begin{aligned} (-axy - bx + cy + e)(V_{xx} - V_{yy}) + [a(x^2 - y^2) - 2by - 2cx - 2d]V_{xy} \\ - 3(ay + b)V_x + 3(ax - c)V_y = 0, \end{aligned} \quad (4.9)$$

$$\phi_x = -2(ay^2 + 2by + d)V_x + 2(axy + bx - cy - e)V_y, \quad (4.10)$$

$$\phi_y = 2(axy + bx - cy - e)V_x + 2(-ax^2 + 2cx + d)V_y. \quad (4.11)$$

Here eq. (4.9) is the compatibility condition for the two equations (4.10) and (4.11). Eq. (4.8) is easily solved.

For  $\alpha \neq 0$  we can translate  $x$  and  $y$  to transform  $\beta \rightarrow 0, \gamma \rightarrow 0$ . Then the potential is rotationally invariant:  $V = V(r)$ .

For  $\alpha = 0, \beta^2 + \gamma^2 \neq 0$  we can rotate to obtain  $\beta \rightarrow 0$ . Then the potential is translationally invariant:  $V = V(x)$ .

To avoid the geometric symmetries (4.7) we solve eq. (4.8) trivially by imposing  $\alpha = \beta = \gamma = 0$ . We then simplify the second order operator  $X$  of eq. (4.5) by rotations, translations and linear combinations with the Hamiltonian  $H$ .

These transformations leave two expressions in the space of the coefficients  $a, \dots, e$  invariant, namely

$$I_1 = a, \quad I_2 = \left[ (2ad - b^2 + c^2)^2 + 4(ae - bc)^2 \right]. \quad (4.12)$$

In the nongeneric case when  $I_1 = I_2 = 0$ , a third invariant exists, namely

$$I_3 = d^2 + e^2. \quad (4.13)$$

Using these invariants, one obtains 4 equivalence classes of operators  $X$  and correspondingly, four classes of potentials allowing for the existence of an operator  $X$ , commuting with the Hamiltonian [3], [5]. The existence of one second order operator  $X$ , satisfying (4.6) makes the system integrable. Moreover, the corresponding Schrödinger equation will allow separation of variables in Cartesian, polar, parabolic or elliptic coordinates, which in the separable system depends on the values of the invariants (4.12) and (4.13).

We are interested in the case of superintegrable Hamiltonians, when two operators  $X_1$  and  $X_2$  exist, satisfying

$$[H, X_1] = [H, X_2] = 0, \quad [X_1, X_2] \neq 0. \quad (4.14)$$

Four classes of such potentials exist, each allowing the separation of variables in at least two coordinate systems. The Hamiltonians and corresponding integrals of motion are:

1.

$$\begin{aligned} H_I &= -\frac{1}{2} (\partial_x^2 + \partial_y^2) + \frac{\omega^2}{2} (x^2 + y^2) + \frac{a}{2x^2} + \frac{b}{2y^2}, \\ \widehat{X}_1 &= P_1^2 - P_2^2 - \left[ \omega^2(x^2 - y^2) + \frac{a}{x^2} - \frac{b}{y^2} \right], \\ \widehat{X}_2 &= L_3^2 - \left( \frac{a}{\cos^2 \phi} + \frac{b}{\sin^2 \phi} \right), \\ x &= r \cos \phi, \quad y = r \sin \phi. \end{aligned} \quad (4.15)$$

2.

$$\begin{aligned} H_{II} &= -\frac{1}{2} (\partial_x^2 + \partial_y^2) + \omega^2(2x^2 + \frac{y^2}{2}) + \frac{a}{2y^2} + bx \\ \widehat{X}_1 &= P_1^2 - P_2^2 - \left[ \omega^2(4x^2 - y^2) + bx - \frac{a}{y^2} \right] \\ \widehat{X}_2 &= L_3 P_2 + P_2 L_3 - 2\omega^2 x y^2 + \frac{2ax}{y^2} - by^2 \end{aligned} \quad (4.16)$$

The remaining two systems are best written in parabolic coordinates

$$x = \frac{1}{2} (\xi^2 - \eta^2), \quad y = \xi\eta. \quad (4.17)$$

3.

$$H_{III} = -\frac{1}{2}\frac{1}{\xi^2 + \eta^2} (\partial_\xi^2 + \partial_\eta^2) + \frac{1}{\xi^2 + \eta^2} \left( 2a + \frac{b}{\xi^2} + \frac{c}{\eta^2} \right) \quad (4.18)$$

$$X_1 = L_3^2 - 2(\xi^2 + \eta^2) \left( \frac{b}{\xi^2} + \frac{c}{\eta^2} \right)$$

$$X_2 = L_3 P_2 + P_2 L_3 + \frac{2}{\xi^2 + \eta^2} \left( a(\xi^2 - \eta^2) - b \frac{\eta^2}{\xi^2} + c \frac{\xi^2}{\eta^2} \right).$$

(For  $b = c = 0$ ,  $a \neq 0$  this is the Coulomb atom). The system allows separation of variables in polar and parabolic coordinates (and also in elliptic coordinates).

4.

$$H_{IV} = -\frac{1}{2}\frac{1}{\xi^2 + \eta^2} (\partial_\xi^2 + \partial_\eta^2) + \frac{2a + b\xi + c\eta}{\xi^2 + \eta^2} \quad (4.19)$$

$$\hat{X}_1 = L_3 P_1 + P_1 L_3 + \frac{b\eta(\eta^2 - \xi^2) + c\xi(\xi^2 - \eta^2) - 4a\eta\xi}{(\xi^2 + \eta^2)}$$

$$\hat{X}_2 = L_3 P_2 + P_2 L_3 + 2 \frac{a(\xi^2 - \eta^2) + \eta\xi(c\xi - b\eta)}{(\xi^2 + \eta^2)}$$

The equation separates in two mutually orthogonal parabolic coordinate systems, namely (4.17) and a similar system with  $x$  and  $y$  interchanged.

For  $a \neq 0$ ,  $b = c = 0$  we again obtain the Coulomb atom.

We shall call the systems  $H_I$  and  $H_{II}$  the *generalized isotropic* and *generalized nonisotropic harmonic oscillators*, respectively. Similarly,  $H_{III}$  and  $H_{IV}$  can both be called *generalized Coulomb systems*.

The Schrödinger equations for  $H_{III}$  and  $H_{IV}$  can be rewritten as

$$\left\{ -\frac{1}{2} (\partial_\xi^2 + \partial_\eta^2) - E(\xi^2 + \eta^2) + \frac{b}{2\xi^2} + \frac{c}{2\eta^2} \right\} \psi = -a\psi, \quad (4.20)$$

$$\left\{ -\frac{1}{2} (\partial_\xi^2 + \partial_\eta^2) - E \left[ \left( \xi - \frac{b}{2E} \right)^2 + \left( \eta - \frac{c}{2E} \right)^2 \right] \right\} \psi = \quad (4.21)$$

$$= \left( -2a - \frac{b^2 + c^2}{4E^2} \right) \psi,$$

respectively. Thus, the system  $H_{III}$  is reduced to  $H_I$  with the energy ( $-E$ ) and coupling constant  $\omega^2$  interchanged. The system  $H_{IV}$  is reduced to a "shifted" harmonic oscillator. This interchange of the energy and a coupling constant has been called "metamorphosis of the coupling constant" [49].

## 4.2 Discrete Generalized Harmonic Oscillators

The umbral correspondence immediately provides us with discrete versions of these systems.

Let us first consider the potential  $V_I$  of eq. (4.15). The discrete version of this system is:

$$H_I^D = -\frac{1}{2} (\Delta_x^2 + \Delta_y^2) + \frac{\omega^2}{2} \left[ (x\beta_x)^2 + (y\beta_y)^2 \right] + \frac{a}{2} (x\beta_x)^{-2} + \frac{b}{2} (y\beta_y)^{-2} \quad (4.22)$$

with the integrals of motion

$$X_1 = \left[ -\frac{1}{2} \Delta_x^2 + \omega^2 (x\beta_x)^2 + a (x\beta_x)^{-2} \right] - \left[ -\frac{1}{2} \Delta_y^2 + \omega^2 (y\beta_y)^2 + b (y\beta_y)^{-2} \right] \quad (4.23)$$

and

$$\begin{aligned} X_2 &= (x\beta_x \Delta_y - y\beta_y \Delta_x)^2 \\ &- \left[ a \left( 1 + (x\beta_x)^{-2} (y\beta_y)^2 \right) + b \left( 1 + (x\beta_x)^2 (y\beta_y)^{-2} \right) \right]. \end{aligned} \quad (4.24)$$

Similarly, the discrete version of the system with potential  $V_{II}$  is

$$H_{II}^D = -\frac{1}{2} (\Delta_x^2 + \Delta_y^2) + \omega^2 \left[ 2(x\beta_x)^2 + \frac{1}{2} (y\beta_y)^2 \right] + \frac{a}{2} (y\beta_y)^{-2} + bx\beta_x. \quad (4.25)$$

The second order operators commuting with the Hamiltonian (4.25) are

$$X_1 = \Delta_x^2 - \Delta_y^2 - \left[ \omega^2 \left( 4(x\beta_x)^2 - (y\beta_y)^2 \right) + b(x\beta_x) - a(y\beta_y)^{-2} \right], \quad (4.26)$$

and

$$\begin{aligned} X_2 &= [(y\beta_y) \Delta_x - (x\beta_x) \Delta_y] \Delta_y + \Delta_y [(y\beta_y) \Delta_x - (x\beta_x) \Delta_y] - 2\omega^2 (x\beta_x) (y\beta_y)^2 \\ &+ 2a (x\beta_x) (y\beta_y)^{-2} - b (y\beta_y)^2. \end{aligned} \quad (4.27)$$

### 4.3 Discrete generalized Coulomb potentials

To discretize the systems  $H_{III}$  and  $H_{IV}$  we again use the umbral correspondence, this time using parabolic coordinates. Thus, we replace

$$\partial_\xi \rightarrow \Delta_\xi, \quad \partial_\eta \rightarrow \Delta_\eta, \quad \xi \rightarrow \xi\beta_\xi, \quad \eta \rightarrow \eta\beta_\eta. \quad (4.28)$$

With these replacements it is a simple matter to write the discrete versions of the systems corresponding to the potentials  $V_{III}$  and  $V_{IV}$ . Indeed, we have

$$H_{III} = -\frac{1}{2} \left[ (\xi\beta_\xi)^2 + (\eta\beta_\eta)^2 \right]^{-1} \left[ \Delta_\xi^2 + \Delta_\eta^2 - 4a - 2b(\xi\beta_\xi)^{-2} - 2c(\eta\beta_\eta)^{-2} \right] \quad (4.29)$$

$$X_1 = [(\xi\beta_\xi)\Delta_\eta - (\eta\beta_\eta)\Delta_\xi]^2 - 2 \left[ (\xi\beta_\xi)^2 + (\eta\beta_\eta)^2 \right] \left[ b(\xi\beta_\xi)^{-2} + c(\eta\beta_\eta)^{-2} \right] \quad (4.30)$$

$$X_2 = \left[ (\xi\beta_\xi)^2 + (\eta\beta_\eta)^2 \right]^{-1} \left\{ (\eta\beta_\eta)^2 \Delta_\xi^2 - (\xi\beta_\xi)^2 \Delta_\eta^2 + 2a \left[ (\xi\beta_\xi)^2 - (\eta\beta_\eta)^2 \right] \right. \\ \left. - 2b(\eta\beta_\eta)^2(\xi\beta_\xi)^{-2} + 2c(\xi\beta_\xi)^2(\eta\beta_\eta)^{-2} \right\} \quad (4.31)$$

and

$$H_{IV} = -\frac{1}{2} \left[ (\xi\beta_\xi)^2 + (\eta\beta_\eta)^2 \right]^{-1} \left[ \Delta_\xi^2 + \Delta_\eta^2 - 4a - 2b(\xi\beta_\xi) - 2c(\eta\beta_\eta) \right] \quad (4.32)$$

$$X_1 = \left[ (\xi\beta_\xi)^2 + (\eta\beta_\eta)^2 \right]^{-1} \left\{ (\xi\beta_\xi)(\eta\beta_\eta) (\Delta_\xi^2 + \Delta_\eta^2) + \right. \\ \left. [-b(\eta\beta_\eta) + c(\xi\beta_\xi)] \left[ (\xi\beta_\xi)^2 - (\eta\beta_\eta)^2 \right] - 4a(\xi\beta_\xi)(\eta\beta_\eta) \right\} - \Delta_{\xi\eta}^2. \quad (4.33)$$

$$X_2 = \frac{1}{2} \left[ (\xi\beta_\xi)^2 + (\eta\beta_\eta)^2 \right]^{-1} \left\{ (\eta\beta_\eta)^2 \Delta_\xi^2 - (\xi\beta_\xi)^2 \Delta_\eta^2 + 2a \left[ (\xi\beta_\xi)^2 - (\eta\beta_\eta)^2 \right] \right. \\ \left. + 2(\xi\beta_\xi)(\eta\beta_\eta) [c(\xi\beta_\xi) - b(\eta\beta_\eta)] \right\} \quad (4.34)$$

## 5 Exact Solvability and Spectral Properties of Discrete Superintegrable Systems

We have shown that certain important properties of the Schrödinger equation, such as point and generalized symmetries, and hence also integrability, are preserved when we pass from continuous to discrete space-time via an umbral correspondence.

Another important property of some quantum systems is their "exact solvability". This means that their Hamiltonian can be transformed into a block diagonal form with finite-dimensional blocks. In other words, their complete energy spectrum can be calculated algebraically. In more mathematical terms, we give the following definition.

**Definition 5.1** *A quantum mechanical system with Hamiltonian  $H$  is called exactly solvable if its Hilbert space  $S$  of bound states consists of a flag of finite dimensional subspaces*

$$S_0 \subset S_1 \subset S_2 \subset \dots S_n \subset \dots \quad (5.1)$$

preserved by the Hamiltonian

$$HS_i \subseteq S_i. \quad (5.2)$$

All known exactly solvable systems also have the following properties.

1. In appropriate coordinates and in an appropriate gauge, the bound state wave functions  $\Psi_N(\vec{x})$  are polynomials:

$$\Psi_N(\vec{x}) = g(\vec{x}) P_N(\vec{s}), \quad s_i = s_i(\vec{x}). \quad (5.3)$$

The gauge factor  $g(\vec{x})$  is a priori defined and can be energy dependent. The function  $P_N(\vec{s})$  are polynomials of order  $N$  in the variables  $s_i$ . The integer  $N$  labels the subspaces  $S_i$  in the flag.

2. In the same gauge  $g$  and same variables  $s_i$  the Hamiltonian  $H$  can be written as

$$H = ghg^{-1}, \quad hP_N = E_N P_N \quad (5.4)$$

with

$$h = a_{ik}^\alpha T_{ik}^\alpha + a_{ik,lm}^{\alpha\beta} T_{ik}^\alpha T_{lm}^\beta \quad (5.5)$$

where  $a_{ik}^\alpha$  and  $a_{ik,lm}^{\alpha\beta}$  are constants (subject to some further conditions [50]) and

$$T_{ik}^\alpha = s_i^\alpha \partial_{s_k}, \quad \alpha = 0, 1, \quad i, k = 1, \dots, n. \quad (5.6)$$

In other words, the gauge rotated Hamiltonian  $h$  is an element of the enveloping algebra of an affine Lie algebra  $aff(n, \mathbb{R})$  (or one of its subalgebras). It is clear that (5.5) guarantees that the Hamiltonian  $H$  will preserve, or decrease the order of the polynomials  $P_N$ . This is a concrete realization of the flag condition (5.2).

We mention that all known quadratically superintegrable systems are exactly solvable, in particular those of Section 4 [6]. For the generalized harmonic oscillators the gauge factor  $g$  is equal to the ground state wave function and is energy independent. The generalized Coulomb systems have been reduced to the harmonic oscillators ones (see (4.20) and (4.21)). However, due to the interchange of the energy and the coupling constant, the gauge factor  $g$  will be energy dependent.

The aim of this Section is to show how exact solvability manifests itself in discrete space-time. First of all, let us consider an arbitrary one-dimensional linear spectral problem

$$L(\partial_x, x)\psi(x) = \lambda\psi(x). \quad (5.7)$$

Let  $x = 0$  be a regular point of this equation. Then any solution can be expanded into a Taylor series

$$\psi(x) = \sum_{k=0}^{\infty} a_k x^k. \quad (5.8)$$

Using the umbral correspondence we write the umbral equation

$$L(\Delta, x\beta)\psi(x\beta) = \lambda\psi(x\beta) \quad (5.9)$$

with the same eigenvalue  $\lambda$  as in the ODE (5.7). Viewed as a difference equation, eq. (5.9) will have a formal power series solution

$$\psi(x\beta)1 = \sum_{k=0}^{\infty} a_k^k (x\beta)^k \cdot 1. \quad (5.10)$$

In particular, if (5.8) is a polynomial solution, then eq. (5.10) will also be a finite sum of terms involving the basic polynomials of the operator  $\Delta$ . Thus, (5.10) will also be a polynomial and all convergence problems disappear.

Now let us turn to the specific case of the generalized harmonic oscillator system with Hamiltonian  $H_I$  (see eq. 4.15) and its discretization (4.22). The

gauge factor  $g$  of eq. (5.3) and (5.4) is

$$g = x^{p_1} y^{p_2} \exp \left[ -\frac{\omega(x^2 + y^2)}{2} \right], \quad a = p_1(p_1 - 1), \quad b = p_2(p_2 - 1). \quad (5.11)$$

We put  $\omega x^2 = s_1$ ,  $\omega y^2 = s_2$  and in these variables the  $aff(2, \mathbb{R})$  operators of eq. (5.6) reduce to

$$\begin{aligned} J_1 &= \partial_{s_1}, & J_2 &= \partial_{s_2}, & J_3 &= s_1 \partial_{s_1}, & J_4 &= s_2 \partial_{s_2}, \\ J_5 &= s_2 \partial_{s_1}, & J_6 &= s_1 \partial_{s_2}. \end{aligned} \quad (5.12)$$

The gauge rotated hamiltonian  $h$  and gauge rotated integrals of motion  $\widehat{x}_1 = g \widehat{X}_1 g^{-1}$ ,  $\widehat{x}_2 = g \widehat{X}_2 g^{-1}$  can now be written as [6]

$$\begin{aligned} h &= -2J_3 J_1 - 2J_4 J_2 + 2J_3 + 2J_4 - (2p_1 + 1) J_1 - (2p_2 + 1) J_2 \\ \widehat{x}_1 &= 2J_3 J_1 - 2J_4 J_2 - 2J_3 + 2J_4 + (2p_1 + 1) J_1 - (2p_2 + 1) J_2 \\ \widehat{x}_2 &= 4J_3 J_5 + 4J_4 J_6 - 8J_3 J_4 + 2(2p_1 + 1) J_5 - 2(2p_2 + 1) J_3 + \\ &\quad - 2(2p_1 + 1) J_4 + 2(2p_2 + 1) J_6. \end{aligned} \quad (5.13)$$

By construction, all three of these operators will conserve the flag of polynomials

$$P_n(s_1, s_2) = \langle (s_1)^{N_1} (s_2)^{N_2} \mid 0 \leq N_1 + N_2 \leq n \rangle \quad (5.14)$$

and this is the reason why the superintegrable system with Hamiltonian  $H_I$  is exactly solvable. The actual solutions of eq. (5.4) are Laguerre polynomials:

$$HP_{nm} = E_{nm} P_{nm}, \quad E_{mn} = n + m, \quad (5.15)$$

$$P_{nm}(x, y) = L_n^{(-1/2+p_1)}(\omega x^2) L_m^{(-1/2+p_2)}(\omega y^2).$$

The umbral discretization will preserve the above properties and will give umbral Laguerre polynomial expressed in terms of  $x\beta_x$  and  $y\beta_y$ . The algebra  $aff(2, \mathbb{R})$  is represented by difference operators

$$\begin{aligned} \widetilde{J}_1 &= \Delta_{s_1}, & \widetilde{J}_2 &= \Delta_{s_2}, & \widetilde{J}_3 &= (s_1 \beta_1) \Delta_{s_1}, & \widetilde{J}_4 &= (s_2 \beta_2) \Delta_{s_2}, \\ \widetilde{J}_5 &= (s_2 \beta_2) \Delta_{s_1}, & \widetilde{J}_6 &= (s_1 \beta_1) \Delta_{s_2}. \end{aligned} \quad (5.16)$$

The formulas (5.13) remain the same (with  $J_i \rightarrow \widetilde{J}_i$ ) and all commutation relations are preserved, as are polynomial solutions. For similar results formulated in terms of operators acting in Fock spaces and the notion of isospectral discretization see Turbiner et al. ([19]–[24]), and [17] for further discussions.

## 6 Conclusions

Much, if not all of nonrelativistic quantum mechanics can be viewed as the "theory of the enveloping algebra of the Heisenberg algebra".

Indeed, let us define the Heisenberg algebra  $H_n$  by the relations

$$[X_j, Y_k] = \delta_{jk}C \quad j, k = 1, \dots, n \quad (6.1)$$

and then put

$$X_j = x_j, \quad Y_k = -i\hbar\partial_{x_k}, \quad C = i\hbar. \quad (6.2)$$

We can say that all quantum mechanical operators lie in the enveloping algebra of  $H_n$ , or in an extension of the enveloping algebra obtained by adding all formal power series in  $x_1, \dots, x_n, p_1, \dots, p_n$ .

If we replace the coordinates  $x_j$  and the momenta  $p_j$  by some other quantities satisfying the relations (6.1) then all polynomials and all power series in these objects will commute in the same way as the corresponding quantum mechanical quantities.

Indeed, the umbral correspondence  $x_i \rightarrow x_i\beta_i$ ,  $\partial_{x_i} \rightarrow \Delta_{x_i}$  preserves the commutation relations (6.1) between quantum mechanical operators. Thus, the umbral correspondence allows us to consider quantum mechanics on a lattice and to preserve all properties of quantum mechanics in continuous space and time that are expressed in terms of the commutation properties of physical quantities (quantum mechanical operators). In particular, infinitesimal point symmetries are preserved, as shown in Sections 3 and 4, respectively. Exact solvability is reduced to an algebraic property and then discretized in Section 5 (and also in the papers [20], [23]–[24]).

Some nonalgebraic properties are lost in the discretization. For instance, the "umbral vector fields" (2.29), obtained by the umbral correspondence, do not generate global transformations (like rotations, or dilations). The solutions of umbral equations (obtained by the umbral correspondence) are often formal, i.e. they may diverge.

The physical content of this article is based on the results contained in Section 2, where we presented and proved several theorems that, to our knowledge, extend the previously known umbral formalism to linear difference equations. In particular we associate with a linear differential equation an abstract operator equation, written in terms of delta operators, using the umbral correspondence (2.23). Any representation of  $\Delta$  and  $\beta$  in terms of shift-invariant operators provides a difference equation, whose analytic solutions can be obtained from the solutions  $\hat{f}$  of the operator equation (2.50)

via the projection  $\hat{f} \cdot 1 = f(x\beta) \cdot 1$ . These are the umbral solutions admitted by a given difference equation. The other possible solutions do not have a continuous limit and are not provided by the umbral approach.

Many of the results presented here can be considered also in the case of  $q$ -difference operators [51]. The delta operator  $U$  in this case is defined in terms of a  $q$ -shift operator satisfying

$$T_q f(x) = f(qx). \quad (6.3)$$

In the simplest case, the  $q$ -difference operator reads

$$\Delta_q = \frac{1}{(q-1)x} (T_q - 1), \quad \lim_{q \rightarrow 1} \Delta_q f = f_x \quad (6.4)$$

and its conjugate operator, obtained imposing the Heisenberg commutation relation

$$[\Delta_q, x\beta_q] = 1 \quad (6.5)$$

is written in terms of a  $q$ -shift and differential operators as

$$\beta_q = (q-1)(qT-1)^{-1} x\partial_x. \quad (6.6)$$

In this case we can still consider the umbral correspondence, but the  $\Delta_q$  operator is not a shift invariant operator, as  $[\Delta_q, T_q] \neq 0$ .

Among open questions, presently under consideration, we mention the following.

- The umbral correspondence has lead us to various linear umbral equations and difference equations. It would be of considerable interest to study their solutions directly and in the case of polynomial solutions, establish their relation to orthogonal polynomials of discrete variables, known in the literature [11], [52].
- Although many of the results presented in this paper can also be carried out in the  $q$ -difference case [51], [53], [54], a reformulation of the umbral theory in this case is necessary.
- The simultaneous diagonalization of commuting sets of second order differential operators is intimately related to the separation of variables in the Schrödinger equation. It would be important to investigate common solutions of commuting sets of difference operators from this point of view.

- A related problem is that of establishing a connection between umbral formalisms introduced in different coordinate systems, e.g. the cartesian quantities  $\Delta_x$ ,  $\Delta_y$ ,  $\beta_x$ ,  $\beta_y$  and the corresponding polar ones, or parabolic ones  $\Delta_\xi$ ,  $\Delta_\eta$ ,  $\beta_\xi$ ,  $\beta_\eta$  introduced in Sections 4 and 5.

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